1,1,1,3,3,3-Hexafluoro-2-propanol

920-66-1 | DTXSID1022134

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.40

Global applicability domain: Outside

Local applicability domain index: 2.78e-01

Confidence level: 7.21e-01

Nearest Neighbors from the Training Set

Image not found
1,1,1,3,3,3-Hexafluoro-2-propanol
Measured: 2.51
Predicted: 2.40

Image not found
o-Toluenesulfonamide
Measured: 2.57
Predicted: 2.00

Image not found
Benzenesulfonamide
Measured: 4.79
Predicted: 2.10

Image not found
Cyanuric acid
Measured: 5.01e-01
Predicted: 1.72

Image not found
Triallyl phosphate
Measured: 1.20
Predicted: 1.41